SCAOT&LANSCE

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tional materials

Shea Mosby holds
a scintillating
crystal, which
when installed
in DANCE (background) lights up
during studies of
radioactive
isotopes.



The one-of-a-kind detector array is ideal for neutron capture measurements on small, radioactive samples.

We are measuring quantities of nature and there is one correct answer—if we have the wherewithal to find it and know that we found it.



Photos by Richard Robinson, IRM-CAS

Shea Mosby

Lighting the way for nuclear science discoveries

By Diana Del Mauro, ADEPS Communications

Cradling a heavy crystal as big as a backyard floodlight, Shea Mosby explained how 160 of these detectors are hidden in a complex device nicknamed the "DANCE ball" at the Lujan Neutron Scattering Center. Together, the detectors form a mass of hexagonal cells in the close-packed sphere, and much of the detector's power derives from this configuration.

Officially named the Detector for Advanced Neutron Capture Experiments, DANCE is a gamma-ray detector array that, when sparked by the intense neutron source at the Los Alamos Neutron Science Center, is ideal for studying nuclear reactions on small, radioactive samples. Mosby's research life as a newly hired Nuclear Science (LANSCE-NS) technical staff member revolves around DANCE, and he supports users as they seek to understand the behavior of radioactive isotopes.

His work crosses applied nuclear physics for defense programs and fundamental nuclear astrophysics for discovery science, a combination that caught his interest when Aaron Couture, now his mentor, made a recruiting trip to Mosby's graduate school.

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From Alex's desk...

When hosting students, please make sure mentoring is a

component of your job.

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Colleagues,

We continue making progress getting ready for the upcoming run cycle, which is due to start in October. Activities are intensifying and we need to be vigilant in planning, preparing, and executing work. In particular, during the summer we host a considerable number of students and visitors (tours included) across all TA-53 activities. When planning a tour, please get familiar with the TA-53 tour policy, found at the following link: mesalib.lanl.gov/87256F35005D1024/All+Documents/1BB194A29F29422087257C7C0 05E185E/\$file/ta53-st-121-001%203-vis-tours_w_sig.pdf. If you have questions, please contact TA53tours@lanl.gov.

When hosting students, please make sure mentoring is a component of your job. Get the students enrolled in the necessary training, make them aware of building locations and surroundings, and plan to meet regularly in their environments. This is all part of making their stay with us productive and an excellent learning experience.

With the Weapons Neutron Research (WNR) proposal call and the Lujan Center-focused proposal call due, we are now about to initiate the proposal science and safety reviews. For this upcoming run cycle, a considerable number of proposals were submitted to both the Lujan and WNR facilities. In a couple of months we plan to have the process finalized and start communicating with users.

Last but not least...enjoy the summer and be safe at home and work, and on travels.

LANSCE Deputy Division Leader Alex H. Lacerda

Mosby cont.

"We are measuring quantities of nature and there is one correct answer—if we have the wherewithal to find it and know that we found it," Mosby said. "Here, there's no answer key." Using DANCE, Mosby and his collaborators are writing it.

In college Mosby earned scholarships, awards, and research fellowships. Yet he faced a steep learning curve at Los Alamos, even though he held a PhD in experimental nuclear physics from Michigan State University, one of the nation's best programs, and cut his teeth at its National Superconducting Cyclotron Laboratory. Mosby had never worked with plutonium, and he said he appreciated how his Los Alamos colleagues gave him time to grapple with the newness. He conversed with some of the Lab's most expert scientists in his field when he and two postdoctoral researchers organized a "Basics of Fission" seminar series for early-career scientists, and he met defense researchers from France who came to DANCE to perform studies impossible anywhere else.

Mosby was surprised when he was asked to help measure the neutron capture cross section of plutonium-239, because he assumed Los Alamos understood this erratic metal when it built the first atomic bomb. DANCE provided a novel method to obtain this measurement despite the large background of gamma rays emitted from neutron-induced fission events. The work was a significant advancement in experimental technique, for which Mosby won a best poster award on Postdoc Research Day. A factor in weapons-related calculations, the cross section also is in demand for Department of Energy advanced nuclear reactor designs.

"Shea brings a broad range of knowledge and skills in modern computing, neutron detection, and nuclear reactions and structure," said instrument scientist John Ullmann. "He couples this with a great deal of enthusiasm and hard work."

Capturing a reaction

"We take neutrons and we throw them into a room," said Mosby, referring figuratively to the accelerator activating an experiment. DANCE then measures the resulting gamma rays emitted when a neutron is captured into the nucleus of the sample being studied. "DANCE can tell you how many gamma rays were emitted, what energy was released in all of them, and where the gamma rays went," he said.

The results appear as those barium-fluoride scintillator crystals—the detectors—light up with a revealing pattern on the sphere. However, "what you hope to see and what you actually see— rarely are the two the same," Mosby said. "You have to understand what you saw to get the physics out."

Light from the detectors, therefore, is converted into electrical signals and transmitted to 15 computers, which glean the most relevant data for analysis. Mosby's latest challenge is testing and refining new computer hardware and software, which will accelerate data processing and replace floor-to-ceiling equipment with a system that could fit in a carry-on suitcase.

Shea Mosby's Favorite Experiment

What: Plutonium-239 capture measurement at DANCE

Why: Plutonium-239's neutron capture cross section is used in defense and nuclear energy applications.

When: February 2013, mostly in the evenings after I helped my wife put our two children to bed.

Where: The Lujan Neutron Scattering Center at LANSCE

Who: Executed with Aaron Couture and John Ullmann. The experimental campaign was a collaboration between LANSCE-NS, Nuclear and Radiochemistry (C-NR), and Lawrence Livermore National Laboratory.

How: A 50-mg sample of plutonium-239 was placed inside DANCE and we analyzed the gamma rays that DANCE observed to measure the neutron capture reaction.

The "a-ha moment:" We got to a preliminary cross section about halfway through the experiment and were able to dig into the details of what we were seeing to observe and diagnose a previously unobserved source of background gamma-ray emission in the measurement. We were then able to slightly modify how we ran the experiment's second half to account for it. A lot of work went into setting up the tools to look at the fine details of our data in almost real-time, and it was very exciting to have it pay off in observing what turned out to be a very subtle effect.

Triphenylmethane: a new neutron moderator?

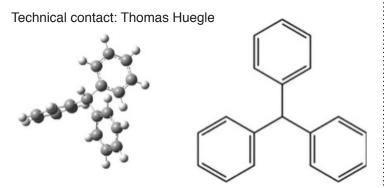
For 40 years, modern spallation neutron sources have used water, liquid hydrogen and liquid methane moderators, each covering one energy range. A material to replace the unstable methane that is also able to operate at a variable energy range is needed to fully utilize high-power neutron sources. In a simultaneous computational and experimental study, Lujan Neutron Scattering Center researchers investigated triphenylmethane, a highly promising candidate as a potential moderator material.

To establish its suitability, the total neutron cross section was experimentally determined at 300 K, 100 K, 10 K; the neutron spectrum was measured on the Filter Difference Spectrometer (FDS); and density functional theory calculations were performed to access excitational modes of the spectrum.

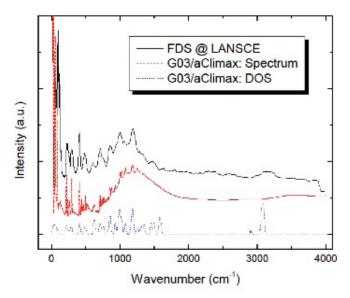
The neutron transmission and spectroscopy measurements agreed with theoretical modeling data, confirming that triphenylmethane meets the requirements for a moderator: three aromatic rings to improve radiation stability, a hydrocarbon structure to mimic the moderating mechanics of methane, and a melting point, which at almost 100 °C means it will not suffer from sudden changes in its moderating capabilities in the temperature range of interest. The next step will be a field test at the Low Energy Neutron Source at Indiana University.

This work, which supports the Laboratory's Energy Security mission and Materials for the Future pillar, benefited from the use of the FDS at Lujan Neutron Scattering Center at LANSCE funded by the DOE Office of Basic Energy Sciences and Los Alamos National Laboratory under DOE Contract DE-AC52-06NA25396.

Reference: "Triphenylmethane, a possible moderator material," by Th. Hügle, M. Mocko, M.A. Hartl, L.L. Daemen, G. Muhrer (all of Lujan Center, LANSCE-LC), *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, **738**, 21 (2014).



Triphenylmethane molecule (left: ball and stick model, right: structure—hydrogen atoms omitted). The three aromatic rings lead to outstanding radiation stability.



Neutron vibrational spectrum (black) and DFT calculation (red). The corresponding density of states (blue) represents the excitational modes that are crucial for neutron moderation.

Measuring the total kinetic energy release in fission

The nuclear fission process consists of a nucleus splitting into two fragments with a significant release of energy. The total kinetic energy of the fission fragments is an important quantity for the understanding and continued development of numerous practical applications, as well as an important constraint on theoretical models of the fission process. Furthermore, the distribution of fission fragment masses is important for nuclear weapons diagnostics as well pro-

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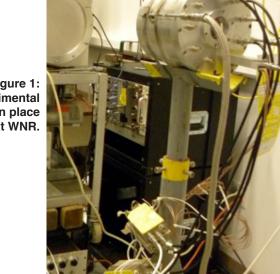


Figure 1: The experimental setup in place at WNR.

Measuring cont.

viding another constraint on theoretical models. Of particular interest is the evolution of these quantities as a function of incident neutron energy, and this energy dependence has historically been poorly constrained. A measurement of these quantities over an unprecedented range of incident neutron energies has been performed on ²³⁵U.

This measurement exploited the neutron beams available at both the Lujan Center and Weapons Neutron Research facility (WNR) at LANSCE. The experimental

technique used the "2E" method to reconstruct the masses and kinetic energies of the fission fragments, which involved measuring each fission fragment's energy deposition in an ionization chamber (see Figure 1). This provided a high efficiency measurement of these quantities with 5 amu mass resolution.

A description of the experimental setup, data acquisition system, and analysis method has been submitted for publication. Figure 2 shows a preliminary fission mass distribution for thermal fission of ²³⁵U compared to evaluation. The expected characteristic structures are seen in the data – in particular the light and heavy mass peaks resulting from asymmetric fission of ²³⁵U. Detailed analysis of both the mass yields and total kinetic energy release as a function of energy is underway.

Figure 3 shows the ²³⁵U fission yields as a function of incident neutron energy for both the Lujan Center and WNR datasets. The high neutron flux that LANSCE delivered combined with the high efficiency of the experimental setup resulted in a dynamic range covering some 11 orders of magnitude incident neutron energy. Such a broad survey is the first of its kind.

A LANL research team including Fredrik Tovesson, Shea Mosby, Dana Duke, Verena Kleinrath, Rhiannon Meharchand, Krista Meierbachtol, Debra Richman, and Daniel Shields (LANSCE-NS) executed the experiment.

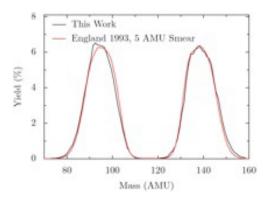


Figure 2: Preliminary mass yields from measurements at LANSCE.

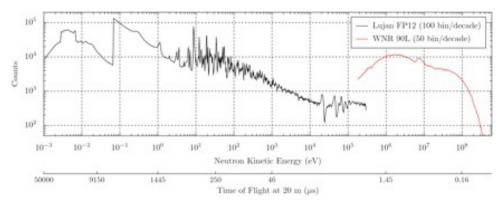


Figure 3: Fission yields as a function of incident neutron energy.

Science Campaign 1 under Stephen Sterbenz funded this experiment, and the results will support the Laboratory's Global Security and Nuclear Deterrence mission areas as well as the Nuclear and Particle Futures science pillar.

Technical Contact: Fredrik Tovesson (or Shea Mosby)

High energy neutron computed tomography at LANSCE

Los Alamos researchers recently developed and demonstrated a unique high-energy neutron computed tomography (n-CT) capability at LANSCE/WNR on Flight Path 15R. This effort is a collaboration between the Non-Destructive Testing and Evaluation Group (AET-6), LANSCE-NS, and Lawrence Livermore National Laboratory (LLNL).

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Figure 4: The high-energy neutron radiography/tomography apparatus on flight path 15R at LANSCE/ WNR. The setup consists of a computer controlled rotating table and a flat panel a-Si detector.

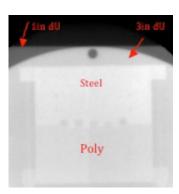




Figure 5: A steel (top half), highdensity polyethylene (bottom half) and foam (center teeth) phantom viewed through 76 mm of depleted uranium. Some ~3-mm diameter holes in the steel are visible.

Tomography cont.

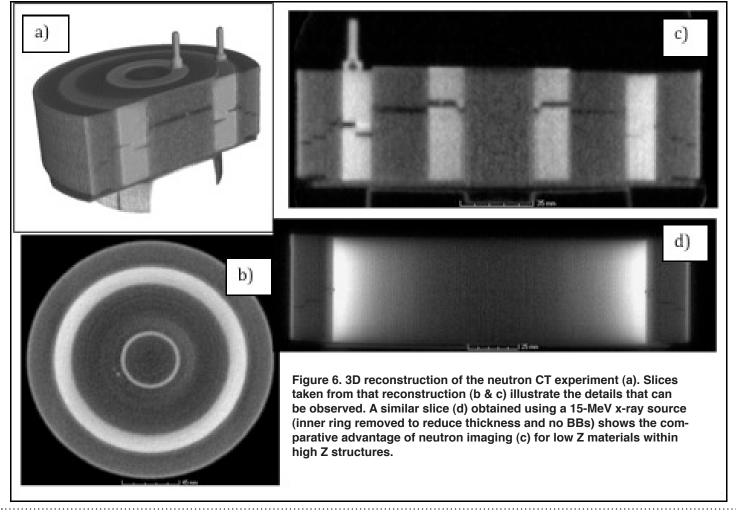
It has long been recognized that neutrons can complement x-rays for imaging. This is due to their very different attenuation characteristics that allow imaging of low Z materials through higher Z materials. For many years, most imaging has been performed with x-rays. One of the main limitations of x-ray imaging is that x-rays are heavily attenuated when passing through dense materials. This absorption increases strongly with atomic number (Z), which limits the ability of x-rays to view low-Z materials obscured by higher Z materials. In addition, x-ray scattering and detection characteristics at high energies make measurement of density profiles and buried feature detection difficult.

For thin items, well established low-energy neutron imaging capabilities are maintained at user facilities like National Institute for Science and Technology and Paul Scherrer Institute. As with x-rays, one reaches a point where higher-energy neutrons are required to penetrate thicker objects. The first high-energy neutron images were obtained in the mid-1990s by LANL (Weapons Neutron Research) and by LLNL (OSU 14-MeV source) with imaging times on the order of 30-60 minute exposures per frame. But these efforts were not used to develop a capability.

During December 2013 and January 2014, a new highenergy neutron imaging capability was demonstrated at LANSCE/WNR on flight path 15R. Figure 4 shows the experimental setup. To show the power of high-energy neutron radiography, the researchers examined two cases.

Figure 5 shows a radiograph of a phantom behind 76 mm of depleted uranium. An 800-viewset experiment of a tungsten and polyethylene test object with 2- and 3-mm tungsten carbide BBs visible in the inner ring (Figure 6) was taken for CT reconstruction using the WNR neutron source. Each view was acquired in less than one minute. Slices taken from that reconstruction (Figures 6b-6c) can be directly compared with an x-ray CT slice of the same object (Figure 6d). It is clear that the neutron imaging shows the internal structure of the object while the x-ray imaging does not show the same detail.

With completion of this demonstration, LANSCE now has a general use high-energy neutron imaging capability that can be deployed on WNR flight paths for unclassified and classified objects. It is anticipated that continued work during the continued on next page



Tomography cont.

next run cycle will improve the speed and resolution of this capability, and the team is considering time-of-flight/energy discrimination as the next major step forward.

Researchers include James Hunter (AET-6), Jim Hall (LLNL), and Ron Nelson (LANSCE-NS). Primary funding for this work is through the Enhanced Surveillance Campaign, and capability development funding was provided by PAD-STE via a Small Equipment Grant. The LANSCE accelerator and neutron sources are funded by RTBF. This work supports the Lab's Nuclear Deterrent and Global Security mission areas and the Science of Signatures and Nuclear and Particle Futures science pillars.

Technical contacts: James Hunter (AET-6) and Ron Nelson (LANSCE-NS)

Neutron scattering enables structural characterization of multifunctional materials

Researchers have discovered a new structure type in a transition metal oxide at the Lujan Neutron Scattering Center. The material has potential applications as a solid oxide fuel cell for clean energy production and as a multiferroic material for computer memory applications. The paper, coauthored by Graham King and Anna Llobet (Lujan Center, LANSCE-LC) and collaborators, was published online in the journal *Advanced Functional Materials*.

The team used neutron powder diffraction with the Lujan Center's high-intensity powder diffractometer (HIPD) instrument as well as electron diffraction to identify a new pattern of charge ordering in TbBaMn $_2$ O $_{5.75}$ and GdBaMn $_2$ O $_{5.75}$. This charge ordering, combined with the layered ordering of the Tb and Ba cations, results in a polar crystal structure. The combination of a non-centrosymmetric space group and magnetic ions makes this a potential multiferroic material. Because the polarization of the material is directly related to the charge ordering of the magnetic ions, strong magnetoelectric coupling can also be

Top: The crystal structure of these materials with the charge ordering pattern highlighted (left) and the exit wave reconstruction data reveal vacancies only within the TbO layer (right). Bottom: The neutron powder diffraction pattern (left) showing supercell reflections resulting from the superstructure and the neutron pair distribution function (right)that gives information on the bond lengths indicate where the oxygen vacancies are located.

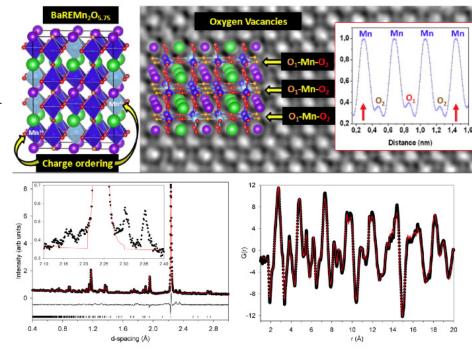
expected. Such materials are rare but greatly sought after by the computer industry.

This material has potential as an ionic conductor for solid oxide fuel cells. Exit wave reconstruction imaging directly imaged the vacancies in the TbO layer. Direct imaging of light atoms, such as oxygen, in the presence of much heavier atoms is very difficult and has only been achieved in a few prior cases. Such imaging can reveal the locations of the vacancies and the mechanism of ionic conduction. Neutron pair distribution function analysis confirmed the ordering of vacancies within the TbO layer. The complementary analytical techniques provided information that enabled the researchers to propose a new model of charge ordering and anion vacancies ordering in these manganites.

Reference: "Structural Determination and Imaging of Charge Ordering and Oxygen Vacancies of the Multifunctional Oxides REBaMn $_2$ O $_{6-\delta}$ (RE = Gd, Tb)," *Advanced Functional Materials*, published online; doi: 10.1002/adfm.201303564. Researchers include G. King and A. Llobet (LANSCE-LC), D. Avila-Brande, E. Urones-Garrote, Subakti, and S. Garcia-Martin (Universidad Complutense de Madrid, Spain).

This work benefited from the use of HIPD at Lujan Center at LANSCE funded by the DOE Office of Basic Energy Sciences.

Technical contact: Graham King



HeadsUP!

P2 recipients recognized for environmental successes

In the spirit of the Directorate's Environmental Action Plan, six members of ADEPS received Pollution Prevention (P2) Awards for their efforts in cleaning the past, controlling the present, and creating a sustainable future. The awards are just one way to document, record, and report significant actions that positively affect the environment.

"Be out of my lab"

Manny Chavez, Dom Peterson, and Gerald Rivera (Polymers & Coatings, MST-7) were part of a five-member team that won a bronze award in the Health and the Environment category. In a complex process requiring special measures, the team removed more than 10 cubic meters of beryllium-contaminated waste and 55 gallons of contaminated equipment from a laboratory, freeing up the space for non-beryllium operations. Removing the beryllium improved the Safety Basis of the facility and reduced the potential exposure of personnel. Nominated by Darryl Garcia (DSESH-STO FOD, DSESH Science & Technology Operations)

"Out with the old, in with the new!"

Scott Currie, Mark Makela, Todd Womack (Subatomic Physics, P-25) were part of an 18-member team that won a silver award in the Cradle to Cradle-Resource Conservation category. The team replaced a 1950s-era, 4,000-gallon tank of liquid nitrogen at LANSCE that was slowly losing about 30% of its contents. The new tank ensures significant cost savings and enhances safety for the workers in the area. Nominated by Roberto Trujillo (Packaging & Transportation, OS-PT)

Colleagues on the LANSCE mesa also received the following P2 awards.

Celebrating service

Congratulations to the following LANSCE and AOT employees celebrating service anniversaries recently:

John Ullmann, LANSCE-NS	35 years
Fred Shelley, AOT-IC	30 years
Gary Holladay, AOT-OPS	25 years
Daniel Rees, AOT-RFE	25 years
William Roybal, AOT-RFE	25 years
Stacy Maestas, AOT-IC	15 years
Geraldine Barela, LANSCE-LC	10 years
Tom Nakotte, LANSCE-LC	5 years
Debra Richman, LANSCE-NS	5 years
Sarah Robinson, AOT-HPE	5 years
Grey Wilburn, LANSCE-NS	5 years

"LANSCE DI bottle disposal"

James Abernathey and John Eddleman (Mechanical Design Engineering, AOT-MDE) and Casey Lang, Mike McCormick, Steve Morgan, Stephen Porto, Lawrence Quintana, and Robert Rieke (Accelerator Operations, AOT-OPS) were part of an 18-member team that won a silver award in the Integrative Planning & Design category. The team developed a new concrete cask to safely transport for disposal spent, mixed-resin beds from the Lujan Neutron Scattering Center. The new process does not require any road closures, thus saving hundreds of work hours; and activated resin beds can be shipped without delay, drastically minimizing legacy waste buildup. Nominated by Eron Kerstiens (AOT-OPS)

"Moving the mountains at LANSCE"

Linda Zwick (Accelerator Operations & Technology, AOT-DO) was part of a three-member team that won a gold award in the Exceptional Service/Sustainability Champion category. Zwick developed and implemented a monthly salvage in-take effort at LANSCE. The team collects items for salvage or recycling and provides advice on appropriate disposal methods for items no longer needed. Benefits include sale of salvage items and recycling of metal and wood. The team is working on a plan to reduce the number of transportainers at LANSCE used to store spare accelerator parts. Nominated by Martha Zumbro (AOT-DO)

For more information on ADEPS's Environmental Action Plan for FY14, please see hsrasweb.lanl.gov/emsdb/org_list_public.asp. For a complete list of P2 award recipients, see int.lanl.gov/environment/p2/awards/index.shtml.

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To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822, or kkippen@ lanl.gov. For past issues, see lansce.lanl.gov/news/pulse.shtml.



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